Full wwPDB X-ray Structure Validation Report (i)

Aug 5, 2026 – 11:56 AM EDT

PDB ID	:	2D0U / pdb_00002d0u
Title	:	Crystal structure of cyanide bound form of human indoleamine 2,3-dioxygenase
Authors	:	Sugimoto, H.; Oda, S.; Otsuki, T.; Hino, T.; Yoshida, T.; Shiro, Y.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2005-08-08
Resolution	:	3.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

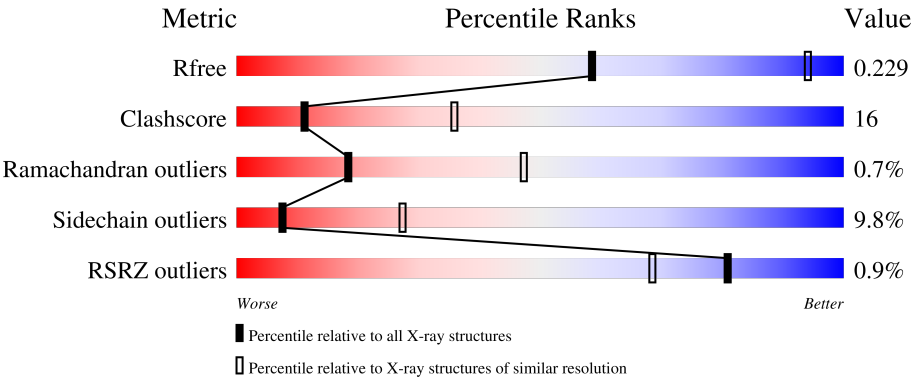
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	406	% 61% 26% • • 8%
1	B	406	% 62% 25% • • 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CYN	A	405	-	-	X	-
2	CYN	B	1405	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6062 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

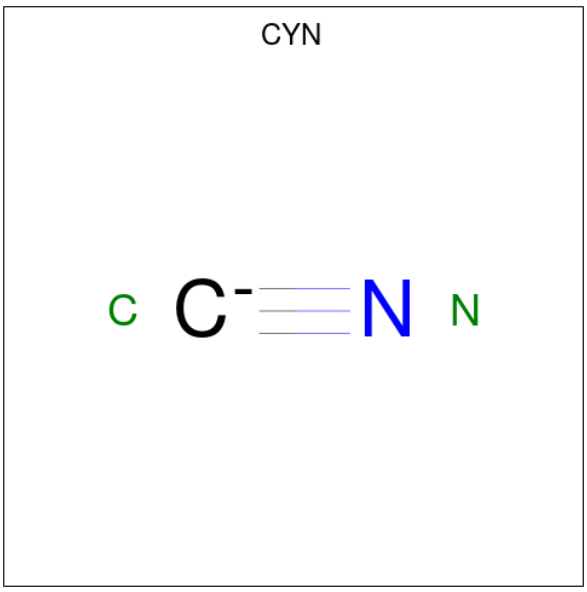
- Molecule 1 is a protein called Indoleamine 2,3-dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	373	Total	C	N	O	S	0	0	0
			2956	1899	504	536	17			
1	B	374	Total	C	N	O	S	0	0	0
			2964	1905	505	537	17			

There are 6 discrepancies between the modelled and reference sequences:

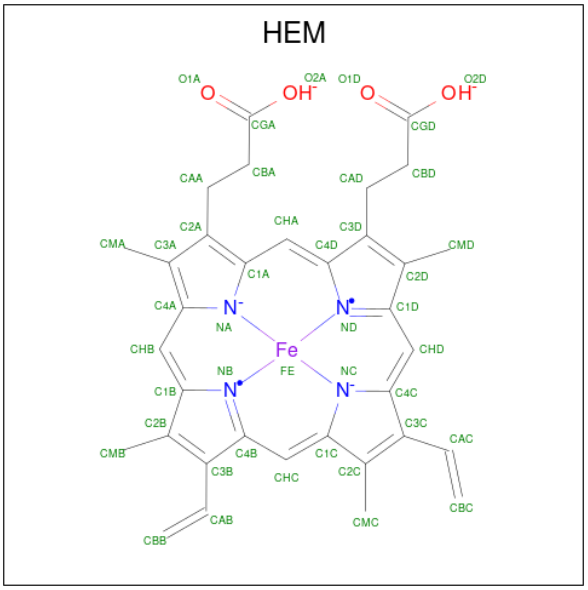
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	cloning artifact	UNP P14902
A	-1	SER	-	cloning artifact	UNP P14902
A	0	HIS	-	cloning artifact	UNP P14902
B	-2	GLY	-	cloning artifact	UNP P14902
B	-1	SER	-	cloning artifact	UNP P14902
B	0	HIS	-	cloning artifact	UNP P14902

- Molecule 2 is CYANIDE ION (CCD ID: CYN) (formula: CN).



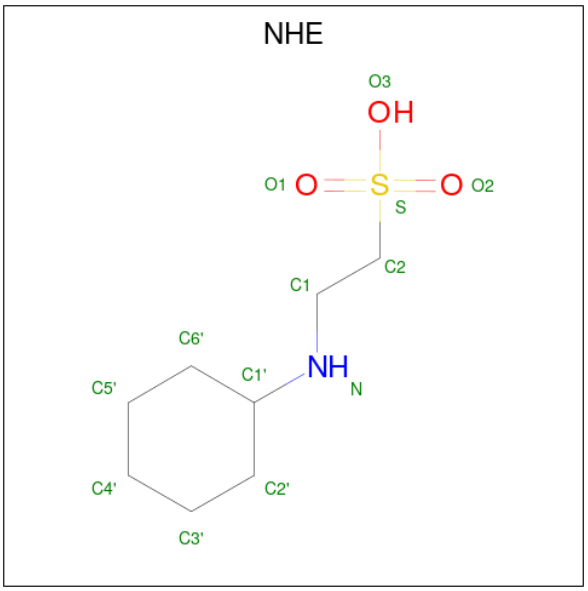
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N 2 1 1	0	0
2	B	1	Total C N 2 1 1	0	0

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C Fe N O 43 34 1 4 4	0	0
3	B	1	Total C Fe N O 43 34 1 4 4	0	0

- Molecule 4 is 2-[N-CYCLOHEXYLAMINO]ETHANE SULFONIC ACID (CCD ID: NHE) (formula: $C_8H_{17}NO_3S$).



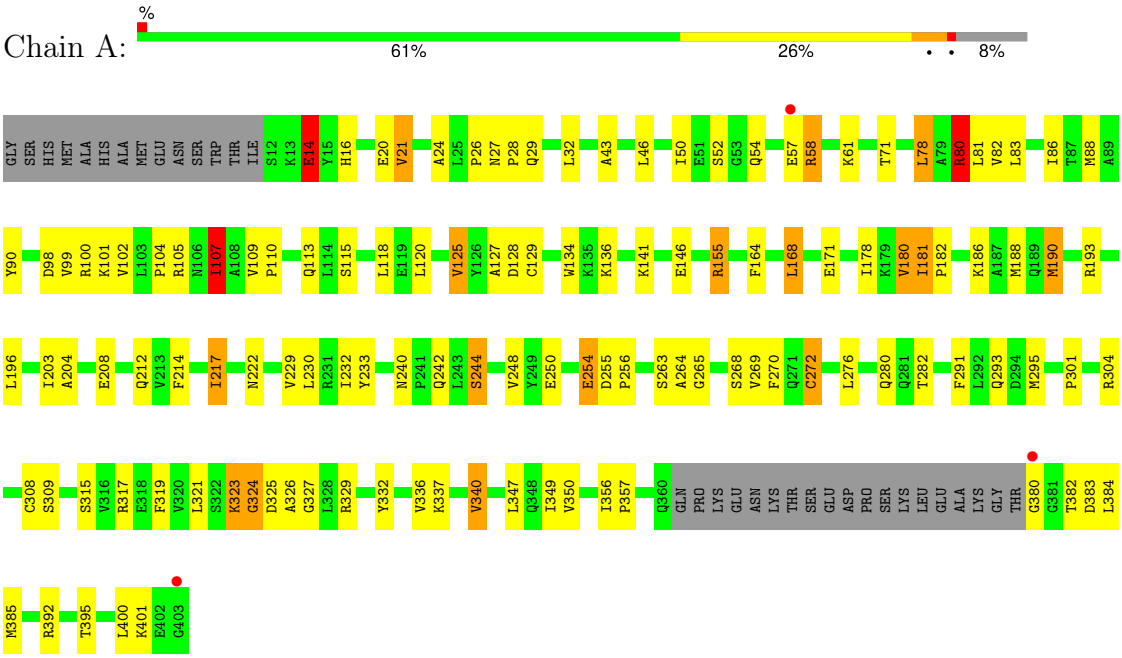
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
4	A	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
4	B	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
4	B	1	Total	C	N	O	S	0	0
			13	8	1	3	1		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

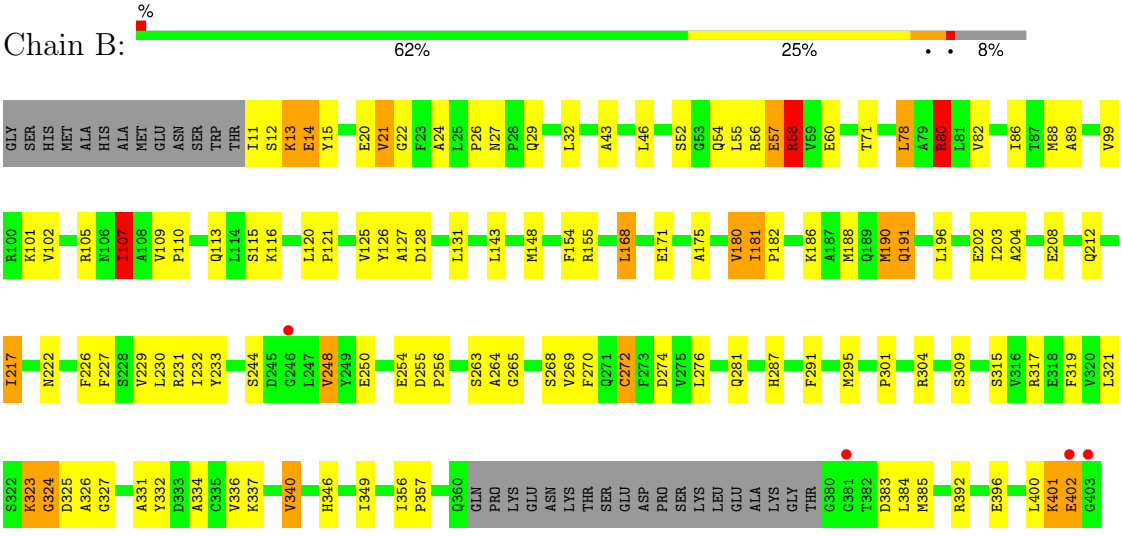
• Molecule 1: Indoleamine 2,3-dioxygenase

Chain A:



• Molecule 1: Indoleamine 2,3-dioxygenase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	86.35Å 97.09Å 129.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.73 – 3.40 19.73 – 3.40	Depositor EDS
% Data completeness (in resolution range)	93.5 (19.73-3.40) 93.0 (19.73-3.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	3.55 (at 3.44Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.213 , 0.254 0.195 , 0.229	Depositor DCC
R_{free} test set	718 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	68.2	Xtriage
Anisotropy	0.445	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 36.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6062	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, NHE, CYN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.66	2/3024 (0.1%)	1.00	6/4087 (0.1%)
1	B	0.66	2/3032 (0.1%)	1.02	10/4098 (0.2%)
All	All	0.66	4/6056 (0.1%)	1.01	16/8185 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	323	LYS	C-O	-13.45	1.07	1.24
1	B	323	LYS	C-O	-12.01	1.07	1.23
1	A	80	ARG	CZ-NH1	-5.95	1.24	1.32
1	B	80	ARG	CZ-NH1	-5.73	1.24	1.32

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	71	THR	N-CA-C	10.09	122.04	111.14
1	B	71	THR	N-CA-C	9.86	121.78	111.14
1	B	401	LYS	N-CA-C	9.15	119.97	108.45
1	B	15	TYR	N-CA-C	-7.13	104.19	113.17
1	B	315	SER	N-CA-C	6.66	119.38	109.59
1	A	315	SER	N-CA-C	6.57	119.25	109.59
1	B	383	ASP	N-CA-C	-6.28	104.49	111.71
1	B	323	LYS	CB-CA-C	-6.22	102.62	111.76
1	B	58	ARG	NE-CZ-NH1	-5.85	115.65	121.50
1	B	323	LYS	O-C-N	-5.62	115.51	122.82
1	A	107	ILE	N-CA-C	-5.31	107.60	111.90
1	A	383	ASP	N-CA-C	-5.27	105.65	111.71
1	A	323	LYS	O-C-N	-5.27	115.59	122.59
1	B	181	ILE	CB-CA-C	-5.13	108.83	113.70
1	A	181	ILE	CB-CA-C	-5.12	108.84	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	107	ILE	N-CA-C	-5.12	107.76	111.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2956	0	2967	107	1
1	B	2964	0	2978	88	1
2	A	2	0	0	2	0
2	B	2	0	0	2	0
3	A	43	0	30	4	0
3	B	43	0	30	4	0
4	A	26	0	32	6	0
4	B	26	0	32	4	0
All	All	6062	0	6069	198	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (198) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:402:GLU:O	1:B:402:GLU:HG3	1.46	1.11
1:B:323:LYS:O	1:B:325:ASP:N	2.00	0.95
1:B:401:LYS:HG2	1:B:402:GLU:H	1.31	0.94
1:B:21:VAL:HG13	1:B:24:ALA:HB3	1.50	0.90
1:A:401:LYS:HE2	1:A:401:LYS:HA	1.55	0.88
1:B:401:LYS:HG2	1:B:402:GLU:N	1.87	0.88
1:B:401:LYS:CG	1:B:402:GLU:H	1.89	0.86
1:A:323:LYS:O	1:A:325:ASP:N	2.09	0.84
1:A:58:ARG:HG3	1:A:58:ARG:HH11	1.43	0.83
1:B:80:ARG:NH2	1:B:121:PRO:O	2.11	0.83
1:A:21:VAL:HG13	1:A:24:ALA:HB3	1.57	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:405:CYN:N	4:A:406:NHE:H5'2	1.93	0.82
1:B:105:ARG:HB3	1:B:250:GLU:HG2	1.62	0.81
1:A:217:ILE:HG21	1:A:349:ILE:HD13	1.62	0.81
1:A:188:MET:HG2	1:A:319:PHE:CD2	2.17	0.80
1:B:88:MET:HE3	1:B:233:TYR:O	1.85	0.77
1:B:13:LYS:HD2	1:B:14:GLU:H	1.47	0.76
1:A:263:SER:CB	4:A:406:NHE:H6'1	2.15	0.75
1:A:264:ALA:HB3	2:A:405:CYN:C	2.17	0.74
1:B:226:PHE:HZ	4:B:1406:NHE:H4'2	1.52	0.74
1:B:102:VAL:HG22	1:B:248:VAL:HG11	1.71	0.73
1:A:136:LYS:HE2	1:A:141:LYS:O	1.88	0.72
1:A:323:LYS:O	1:A:324:GLY:C	2.32	0.69
1:B:21:VAL:CG1	1:B:24:ALA:HB3	2.22	0.68
1:A:28:PRO:HG2	1:A:134:TRP:O	1.93	0.67
1:B:287:HIS:CE1	4:B:1407:NHE:H4'2	2.28	0.67
1:B:356:ILE:HB	1:B:357:PRO:HD3	1.76	0.67
1:B:255:ASP:HB3	1:B:256:PRO:HD2	1.76	0.67
1:A:190:MET:HA	1:A:190:MET:HE2	1.77	0.67
1:A:329:ARG:HE	1:A:401:LYS:HD2	1.60	0.66
1:B:402:GLU:O	1:B:402:GLU:CG	2.30	0.66
1:A:102:VAL:HG22	1:A:248:VAL:HG11	1.76	0.66
1:B:102:VAL:HG22	1:B:248:VAL:CG1	2.26	0.66
1:B:323:LYS:O	1:B:324:GLY:C	2.38	0.65
1:B:52:SER:OG	1:B:54:GLN:HG3	1.97	0.65
1:A:217:ILE:HG21	1:A:349:ILE:CD1	2.26	0.65
1:A:102:VAL:HG22	1:A:248:VAL:CG1	2.27	0.65
1:A:217:ILE:O	1:A:217:ILE:HD13	1.97	0.64
1:A:356:ILE:HB	1:A:357:PRO:HD3	1.79	0.63
1:B:24:ALA:HA	1:B:131:LEU:HD22	1.81	0.62
1:A:14:GLU:C	1:A:16:HIS:H	2.06	0.62
1:A:52:SER:OG	1:A:54:GLN:HG2	2.00	0.62
1:A:27:ASN:O	1:A:27:ASN:ND2	2.33	0.61
1:A:263:SER:HB2	4:A:406:NHE:H6'1	1.82	0.61
1:B:321:LEU:HD21	1:B:400:LEU:HD22	1.82	0.60
1:B:13:LYS:CD	1:B:14:GLU:H	2.15	0.59
1:B:301:PRO:HA	1:B:304:ARG:NH1	2.17	0.59
1:A:329:ARG:NE	1:A:401:LYS:HD2	2.17	0.59
1:A:88:MET:HE3	1:A:233:TYR:O	2.02	0.59
1:A:301:PRO:HA	1:A:304:ARG:NH1	2.17	0.59
1:A:255:ASP:HB3	1:A:256:PRO:HD2	1.85	0.59
1:B:102:VAL:HA	1:B:248:VAL:HG13	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:ARG:O	1:B:60:GLU:HG3	2.03	0.58
1:A:321:LEU:HD21	1:A:400:LEU:HD22	1.85	0.58
1:B:43:ALA:HB2	1:B:82:VAL:HG13	1.86	0.58
1:A:347:LEU:HD12	1:A:392:ARG:HH11	1.68	0.57
1:B:32:LEU:HG	1:B:78:LEU:HD13	1.85	0.57
1:B:171:GLU:OE2	1:B:269:VAL:HG23	2.05	0.57
1:B:217:ILE:HG21	1:B:349:ILE:HD12	1.87	0.57
1:A:58:ARG:HH11	1:A:58:ARG:CG	2.15	0.56
1:B:180:VAL:HG21	1:B:203:ILE:HG13	1.86	0.56
1:B:190:MET:HE3	1:B:190:MET:HA	1.88	0.56
1:A:204:ALA:O	1:A:208:GLU:HG3	2.05	0.55
1:A:21:VAL:CG1	1:A:24:ALA:HB3	2.34	0.55
1:B:384:LEU:HD21	3:B:404:HEM:HMA3	1.88	0.55
1:A:181:ILE:HD12	1:A:276:LEU:HG	1.87	0.55
1:B:11:ILE:HG22	1:B:12:SER:N	2.22	0.54
1:A:21:VAL:HG13	1:A:21:VAL:O	2.05	0.54
1:A:188:MET:HG2	1:A:319:PHE:CE2	2.41	0.54
1:B:57:GLU:HG3	1:B:58:ARG:N	2.16	0.54
1:B:107:ILE:O	1:B:110:PRO:HD2	2.08	0.54
1:A:254:GLU:H	1:A:254:GLU:CD	2.15	0.54
1:A:58:ARG:CG	1:A:58:ARG:NH1	2.70	0.53
1:A:190:MET:HA	1:A:190:MET:CE	2.38	0.53
1:A:171:GLU:OE2	1:A:269:VAL:HG23	2.09	0.53
1:A:317:ARG:HD2	1:A:332:TYR:OH	2.08	0.53
4:A:406:NHE:HC21	4:A:407:NHE:HN	1.73	0.53
1:B:317:ARG:HD2	1:B:332:TYR:OH	2.08	0.53
1:A:269:VAL:HG12	1:A:270:PHE:CD1	2.43	0.53
1:B:287:HIS:HE1	4:B:1407:NHE:H4'2	1.71	0.53
1:B:384:LEU:HD11	3:B:404:HEM:HMA3	1.91	0.53
1:A:80:ARG:HG3	1:A:118:LEU:HD12	1.90	0.53
1:A:181:ILE:HB	1:A:182:PRO:HD3	1.91	0.53
1:A:180:VAL:HG21	1:A:203:ILE:HG13	1.90	0.52
1:A:263:SER:HA	4:A:406:NHE:H6'1	1.90	0.52
1:A:263:SER:CA	4:A:406:NHE:H6'1	2.39	0.52
1:A:101:LYS:O	1:A:248:VAL:HG12	2.10	0.52
1:B:155:ARG:HD2	1:B:233:TYR:OH	2.10	0.52
1:A:268:SER:O	1:A:272:CYS:HB3	2.10	0.52
1:A:295:MET:HA	1:A:295:MET:HE2	1.90	0.52
1:B:14:GLU:N	1:B:14:GLU:CD	2.68	0.52
1:A:14:GLU:C	1:A:14:GLU:CD	2.78	0.51
1:B:101:LYS:O	1:B:248:VAL:HG12	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:MET:HG2	1:B:319:PHE:CD2	2.46	0.51
1:B:385:MET:HA	1:B:385:MET:HE2	1.93	0.51
1:B:109:VAL:O	1:B:113:GLN:HG3	2.10	0.51
1:B:127:ALA:HA	1:B:131:LEU:HD12	1.93	0.51
1:B:82:VAL:O	1:B:86:ILE:HG13	2.11	0.50
1:A:350:VAL:HG11	1:A:385:MET:HE1	1.93	0.50
1:A:32:LEU:HG	1:A:78:LEU:HD13	1.92	0.50
1:A:384:LEU:HD11	3:A:404:HEM:HMA3	1.94	0.50
1:A:109:VAL:HB	1:A:110:PRO:HD3	1.94	0.50
1:B:168:LEU:O	1:B:171:GLU:HB3	2.12	0.50
1:A:58:ARG:HG3	1:A:58:ARG:NH1	2.17	0.50
1:A:269:VAL:HG12	1:A:270:PHE:HD1	1.77	0.50
1:B:181:ILE:HB	1:B:182:PRO:HD3	1.94	0.50
1:B:29:GLN:O	1:B:78:LEU:HG	2.12	0.49
1:A:105:ARG:HB3	1:A:250:GLU:HG2	1.93	0.49
1:A:350:VAL:HG11	1:A:385:MET:CE	2.43	0.49
1:A:384:LEU:HD11	3:A:404:HEM:CMA	2.42	0.49
1:A:282:THR:CG2	1:A:293:GLN:OE1	2.60	0.49
1:B:268:SER:O	1:B:272:CYS:HB3	2.13	0.48
1:B:143:LEU:HD22	1:B:148:MET:HE3	1.96	0.48
1:B:270:PHE:CD1	1:B:270:PHE:N	2.81	0.48
1:A:115:SER:HB3	1:A:120:LEU:O	2.14	0.48
1:A:29:GLN:O	1:A:78:LEU:HG	2.14	0.48
1:A:43:ALA:HB2	1:A:82:VAL:HG13	1.96	0.48
1:B:191:GLN:HE21	1:B:191:GLN:CA	2.26	0.48
1:B:154:PHE:O	1:B:155:ARG:HG2	2.14	0.47
1:B:336:VAL:O	1:B:340:VAL:HG13	2.14	0.47
1:B:21:VAL:HG13	1:B:21:VAL:O	2.14	0.47
1:B:109:VAL:HB	1:B:110:PRO:HD3	1.96	0.47
1:A:384:LEU:HD21	3:A:404:HEM:HMA3	1.95	0.47
1:A:107:ILE:O	1:A:110:PRO:HD2	2.13	0.47
1:B:269:VAL:HG12	1:B:270:PHE:CD1	2.49	0.47
1:A:214:PHE:CE1	1:A:349:ILE:HD12	2.49	0.47
1:B:384:LEU:HD11	3:B:404:HEM:CMA	2.45	0.47
1:A:282:THR:HG21	1:A:293:GLN:OE1	2.15	0.47
1:A:401:LYS:HE2	1:A:401:LYS:CA	2.37	0.47
1:A:102:VAL:HA	1:A:248:VAL:HG13	1.96	0.46
1:A:80:ARG:NH2	1:A:128:ASP:OD2	2.46	0.46
1:A:269:VAL:HG12	1:A:270:PHE:N	2.30	0.46
1:B:21:VAL:CG1	1:B:21:VAL:O	2.63	0.46
1:B:319:PHE:C	1:B:319:PHE:CD1	2.94	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:SER:HB3	1:B:120:LEU:O	2.15	0.46
1:A:380:GLY:C	1:A:382:THR:H	2.23	0.46
1:A:83:LEU:HD22	1:A:107:ILE:HD11	1.98	0.46
1:B:26:PRO:O	1:B:27:ASN:C	2.58	0.46
1:B:269:VAL:HG12	1:B:270:PHE:N	2.31	0.45
1:A:50:ILE:HG21	1:A:155:ARG:HE	1.78	0.45
1:A:155:ARG:HH11	1:A:155:ARG:HB3	1.81	0.45
1:A:100:ARG:HA	1:A:100:ARG:HD3	1.75	0.45
1:B:204:ALA:O	1:B:208:GLU:HG3	2.16	0.45
1:A:26:PRO:O	1:A:27:ASN:C	2.59	0.45
1:B:191:GLN:HE21	1:B:191:GLN:HA	1.82	0.45
1:B:264:ALA:HB3	2:B:1405:CYN:C	2.47	0.45
1:A:350:VAL:CG1	1:A:385:MET:HE1	2.47	0.45
1:A:282:THR:O	1:A:282:THR:HG22	2.16	0.45
1:B:274:ASP:OD2	1:B:281:GLN:HG3	2.17	0.45
1:A:14:GLU:C	1:A:16:HIS:N	2.73	0.45
3:B:404:HEM:HBA1	4:B:1407:NHE:H6'2	1.99	0.45
1:A:385:MET:HA	1:A:385:MET:HE2	1.99	0.45
1:A:146:GLU:H	1:A:146:GLU:CD	2.24	0.44
1:A:319:PHE:CE1	1:A:323:LYS:HE2	2.52	0.44
1:B:13:LYS:NZ	1:B:14:GLU:HB2	2.32	0.44
1:B:80:ARG:NH1	1:B:128:ASP:OD2	2.51	0.44
1:B:263:SER:C	1:B:265:GLY:N	2.75	0.44
1:A:326:ALA:O	1:A:327:GLY:C	2.61	0.44
1:A:78:LEU:O	1:A:81:LEU:HB3	2.18	0.44
1:A:193:ARG:C	1:A:193:ARG:HD3	2.43	0.44
1:A:263:SER:C	1:A:265:GLY:N	2.75	0.43
1:A:270:PHE:CD1	1:A:270:PHE:N	2.86	0.43
1:A:282:THR:CG2	1:A:282:THR:O	2.66	0.43
1:B:264:ALA:HB3	2:B:1405:CYN:N	2.34	0.43
1:A:336:VAL:O	1:A:340:VAL:HG13	2.18	0.43
1:A:125:VAL:HG13	1:A:127:ALA:H	1.83	0.43
1:B:217:ILE:HD13	1:B:217:ILE:O	2.17	0.43
1:A:98:ASP:OD1	1:A:98:ASP:C	2.61	0.43
1:B:291:PHE:O	1:B:295:MET:HG2	2.18	0.43
1:B:154:PHE:C	1:B:155:ARG:HG2	2.44	0.43
1:A:178:ILE:O	1:A:181:ILE:HG12	2.19	0.43
1:B:27:ASN:O	1:B:27:ASN:ND2	2.52	0.43
1:A:90:TYR:CE2	1:A:104:PRO:HD3	2.53	0.42
1:A:181:ILE:CD1	1:A:276:LEU:HG	2.49	0.42
1:B:126:TYR:CD1	1:B:264:ALA:HA	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:VAL:CG1	1:A:21:VAL:O	2.63	0.42
1:B:346:HIS:O	1:B:349:ILE:HB	2.18	0.42
1:B:326:ALA:O	1:B:327:GLY:C	2.61	0.42
1:B:331:ALA:O	1:B:334:ALA:HB3	2.20	0.42
1:B:229:VAL:O	1:B:232:ILE:HB	2.20	0.42
1:B:55:LEU:HD22	1:B:89:ALA:HB1	2.01	0.42
1:A:82:VAL:O	1:A:86:ILE:HG13	2.19	0.41
1:A:109:VAL:O	1:A:113:GLN:HG3	2.20	0.41
1:A:340:VAL:HG12	1:A:395:THR:HG22	2.02	0.41
1:A:270:PHE:HD1	1:A:270:PHE:N	2.19	0.41
1:B:22:GLY:HA3	1:B:175:ALA:CB	2.50	0.41
1:A:136:LYS:CE	1:A:141:LYS:O	2.65	0.41
1:B:270:PHE:HD1	1:B:270:PHE:H	1.69	0.41
1:A:240:ASN:OD1	1:A:242:GLN:HG2	2.20	0.41
1:B:227:PHE:O	1:B:231:ARG:NH1	2.53	0.41
1:A:146:GLU:CD	1:A:146:GLU:N	2.79	0.40
1:A:168:LEU:O	1:A:171:GLU:HB3	2.20	0.40
1:B:13:LYS:CD	1:B:14:GLU:N	2.83	0.40
1:A:129:CYS:HB2	1:A:164:PHE:CZ	2.56	0.40
1:B:181:ILE:CD1	1:B:276:LEU:HG	2.51	0.40
1:A:384:LEU:HD11	3:A:404:HEM:HAA1	2.03	0.40
1:A:291:PHE:O	1:A:295:MET:HG2	2.21	0.40
1:A:229:VAL:O	1:A:232:ILE:HB	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:ARG:NH2	1:B:402:GLU:OE1[3_655]	2.08	0.12

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	369/406 (91%)	346 (94%)	20 (5%)	3 (1%)	16 44
1	B	370/406 (91%)	349 (94%)	19 (5%)	2 (0%)	24 54
All	All	739/812 (91%)	695 (94%)	39 (5%)	5 (1%)	18 47

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	324	GLY
1	B	324	GLY
1	B	244	SER
1	A	244	SER
1	A	14	GLU

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	322/350 (92%)	292 (91%)	30 (9%)	8 29
1	B	323/350 (92%)	290 (90%)	33 (10%)	7 25
All	All	645/700 (92%)	582 (90%)	63 (10%)	7 27

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLU
1	A	20	GLU
1	A	21	VAL
1	A	46	LEU
1	A	57	GLU
1	A	58	ARG
1	A	61	LYS
1	A	78	LEU
1	A	80	ARG
1	A	99	VAL
1	A	107	ILE

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Mol	Chain	Res	Type
1	A	125	VAL
1	A	155	ARG
1	A	168	LEU
1	A	180	VAL
1	A	186	LYS
1	A	190	MET
1	A	196	LEU
1	A	212	GLN
1	A	217	ILE
1	A	222	ASN
1	A	230	LEU
1	A	244	SER
1	A	254	GLU
1	A	272	CYS
1	A	280	GLN
1	A	308	CYS
1	A	309	SER
1	A	337	LYS
1	A	340	VAL
1	B	13	LYS
1	B	14	GLU
1	B	20	GLU
1	B	21	VAL
1	B	46	LEU
1	B	57	GLU
1	B	58	ARG
1	B	78	LEU
1	B	80	ARG
1	B	99	VAL
1	B	107	ILE
1	B	116	LYS
1	B	125	VAL
1	B	168	LEU
1	B	180	VAL
1	B	186	LYS
1	B	190	MET
1	B	191	GLN
1	B	196	LEU
1	B	202	GLU
1	B	212	GLN
1	B	217	ILE
1	B	222	ASN

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Mol	Chain	Res	Type
1	B	230	LEU
1	B	248	VAL
1	B	254	GLU
1	B	272	CYS
1	B	309	SER
1	B	337	LYS
1	B	340	VAL
1	B	392	ARG
1	B	396	GLU
1	B	402	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	37	ASN
1	A	212	GLN
1	A	242	GLN
1	A	280	GLN
1	B	16	HIS
1	B	37	ASN
1	B	45	HIS
1	B	63	ASN
1	B	191	GLN
1	B	220	HIS
1	B	242	GLN
1	B	287	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	HEM	A	404	1	50,50,50	1.98	12 (24%)	67,82,82	1.34	8 (11%)
2	CYN	A	405	-	1,1,1	0.93	0	-		
2	CYN	B	1405	-	1,1,1	0.88	0	-		
4	NHE	B	1406	-	13,13,13	1.57	1 (7%)	16,17,17	0.98	1 (6%)
4	NHE	B	1407	-	13,13,13	1.47	2 (15%)	16,17,17	0.98	1 (6%)
4	NHE	A	406	-	13,13,13	1.72	1 (7%)	16,17,17	1.02	1 (6%)
4	NHE	A	407	-	13,13,13	1.58	2 (15%)	16,17,17	0.75	0
3	HEM	B	404	1	50,50,50	2.02	16 (32%)	67,82,82	1.45	7 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	A	404	1	-	9/14/54/54	-
4	NHE	B	1406	-	-	2/7/15/15	0/1/1/1
4	NHE	B	1407	-	-	2/7/15/15	0/1/1/1
4	NHE	A	406	-	-	0/7/15/15	0/1/1/1
4	NHE	A	407	-	-	0/7/15/15	0/1/1/1
3	HEM	B	404	1	-	9/14/54/54	-

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	404	HEM	FE-NC	6.88	2.17	1.95
3	B	404	HEM	FE-NC	6.05	2.15	1.95
3	B	404	HEM	FE-NB	6.03	2.13	1.94
4	A	406	NHE	C2-S	-5.48	1.69	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1406	NHE	C2-S	-5.12	1.70	1.77
3	A	404	HEM	FE-NB	5.07	2.10	1.94
4	A	407	NHE	C2-S	-4.35	1.71	1.77
4	B	1407	NHE	C2-S	-4.21	1.71	1.77
3	A	404	HEM	CHD-C4C	4.04	1.46	1.38
3	B	404	HEM	FE-NA	3.27	2.05	1.95
3	A	404	HEM	CHD-C1D	3.07	1.46	1.39
3	B	404	HEM	CAC-C3C	-2.75	1.40	1.47
3	B	404	HEM	CHD-C4C	2.61	1.43	1.38
3	A	404	HEM	FE-NA	2.54	2.03	1.95
3	A	404	HEM	CAC-C3C	-2.54	1.40	1.47
3	B	404	HEM	CBB-CAB	2.51	1.42	1.30
4	A	407	NHE	C1-N	2.51	1.52	1.47
3	A	404	HEM	CBD-CGD	2.46	1.56	1.50
3	A	404	HEM	CBB-CAB	2.46	1.42	1.30
3	A	404	HEM	C4C-NC	-2.46	1.35	1.39
3	B	404	HEM	CAD-C3D	2.42	1.57	1.51
3	B	404	HEM	CMC-C2C	2.41	1.55	1.50
3	B	404	HEM	C1C-NC	-2.40	1.35	1.39
3	B	404	HEM	CMB-C2B	2.37	1.55	1.50
3	A	404	HEM	C1A-NA	-2.36	1.35	1.39
3	B	404	HEM	CBD-CGD	2.34	1.56	1.50
3	B	404	HEM	CMA-C3A	2.30	1.55	1.50
3	B	404	HEM	CBA-CGA	2.26	1.55	1.50
3	B	404	HEM	CHD-C1D	2.23	1.44	1.39
3	A	404	HEM	CMB-C2B	2.23	1.55	1.50
3	A	404	HEM	CAD-C3D	2.14	1.56	1.51
3	B	404	HEM	C4A-NA	-2.12	1.35	1.39
4	B	1407	NHE	C1-N	2.10	1.51	1.47
3	B	404	HEM	CHB-C1B	2.04	1.42	1.38

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	404	HEM	CBD-CAD-C3D	4.51	124.99	112.53
3	B	404	HEM	CAA-CBA-CGA	4.42	125.38	113.67
3	A	404	HEM	CAD-CBD-CGD	4.41	125.35	113.67
3	A	404	HEM	CBD-CAD-C3D	4.37	124.62	112.53
3	B	404	HEM	CBA-CAA-C2A	4.13	123.95	112.53
3	B	404	HEM	CAD-CBD-CGD	4.10	124.53	113.67
3	A	404	HEM	CBA-CAA-C2A	4.05	123.74	112.53
3	A	404	HEM	CAA-CBA-CGA	3.37	122.61	113.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	404	HEM	C4B-C3B-C2B	-2.98	104.54	107.28
3	B	404	HEM	C3B-C4B-NB	2.95	111.59	109.47
4	B	1407	NHE	C2-C1-N	-2.78	103.46	111.40
3	A	404	HEM	C4B-C3B-C2B	-2.70	104.80	107.28
4	A	406	NHE	C2-C1-N	-2.31	104.81	111.40
3	B	404	HEM	C3B-C2B-C1B	2.30	108.14	106.41
4	B	1406	NHE	C1-N-C1'	-2.14	110.06	114.18
3	A	404	HEM	C3B-C2B-C1B	2.09	107.98	106.41
3	A	404	HEM	C3B-C4B-NB	2.02	110.92	109.47
3	A	404	HEM	O2D-CGD-CBD	2.01	120.36	114.00

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	404	HEM	C2C-C3C-CAC-CBC
3	B	404	HEM	C2C-C3C-CAC-CBC
3	A	404	HEM	C2A-CAA-CBA-CGA
3	B	404	HEM	C2A-CAA-CBA-CGA
4	B	1406	NHE	C2'-C1'-N-C1
4	B	1406	NHE	C6'-C1'-N-C1
4	B	1407	NHE	C6'-C1'-N-C1
3	A	404	HEM	C2B-C3B-CAB-CBB
3	B	404	HEM	C2B-C3B-CAB-CBB
3	A	404	HEM	C4C-C3C-CAC-CBC
3	B	404	HEM	C4C-C3C-CAC-CBC
3	A	404	HEM	CAD-CBD-CGD-O1D
3	A	404	HEM	CAA-CBA-CGA-O2A
3	A	404	HEM	CAA-CBA-CGA-O1A
3	B	404	HEM	CAA-CBA-CGA-O1A
4	B	1407	NHE	C2'-C1'-N-C1
3	B	404	HEM	CAD-CBD-CGD-O1D
3	A	404	HEM	CAD-CBD-CGD-O2D
3	B	404	HEM	CAA-CBA-CGA-O2A
3	B	404	HEM	CAD-CBD-CGD-O2D
3	A	404	HEM	C4B-C3B-CAB-CBB
3	B	404	HEM	C4B-C3B-CAB-CBB

There are no ring outliers.

8 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	404	HEM	4	0
2	A	405	CYN	2	0
2	B	1405	CYN	2	0
4	B	1406	NHE	1	0
4	B	1407	NHE	3	0
4	A	406	NHE	6	0
4	A	407	NHE	1	0
3	B	404	HEM	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

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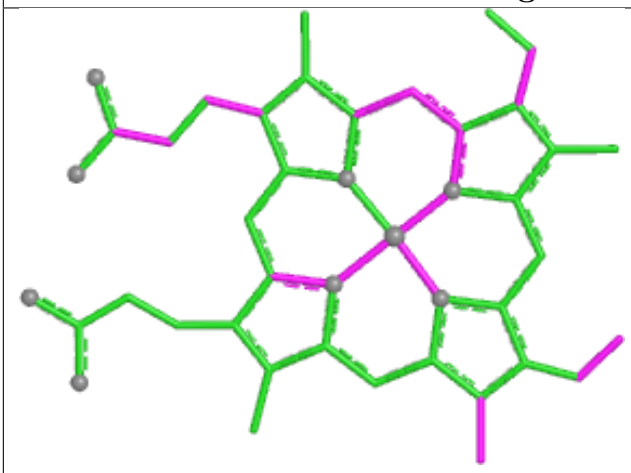
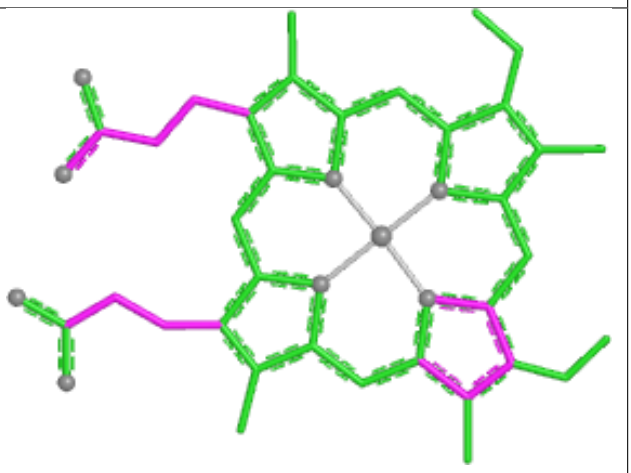
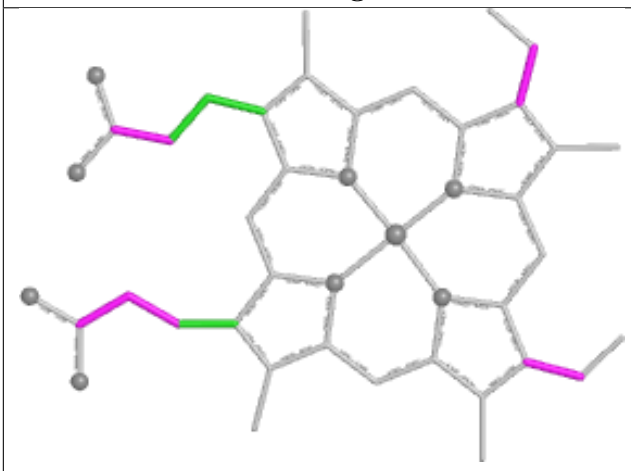


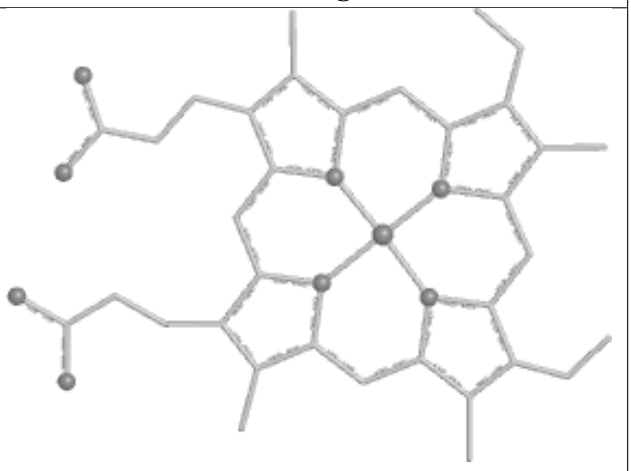
Bond lengths



Bond angles

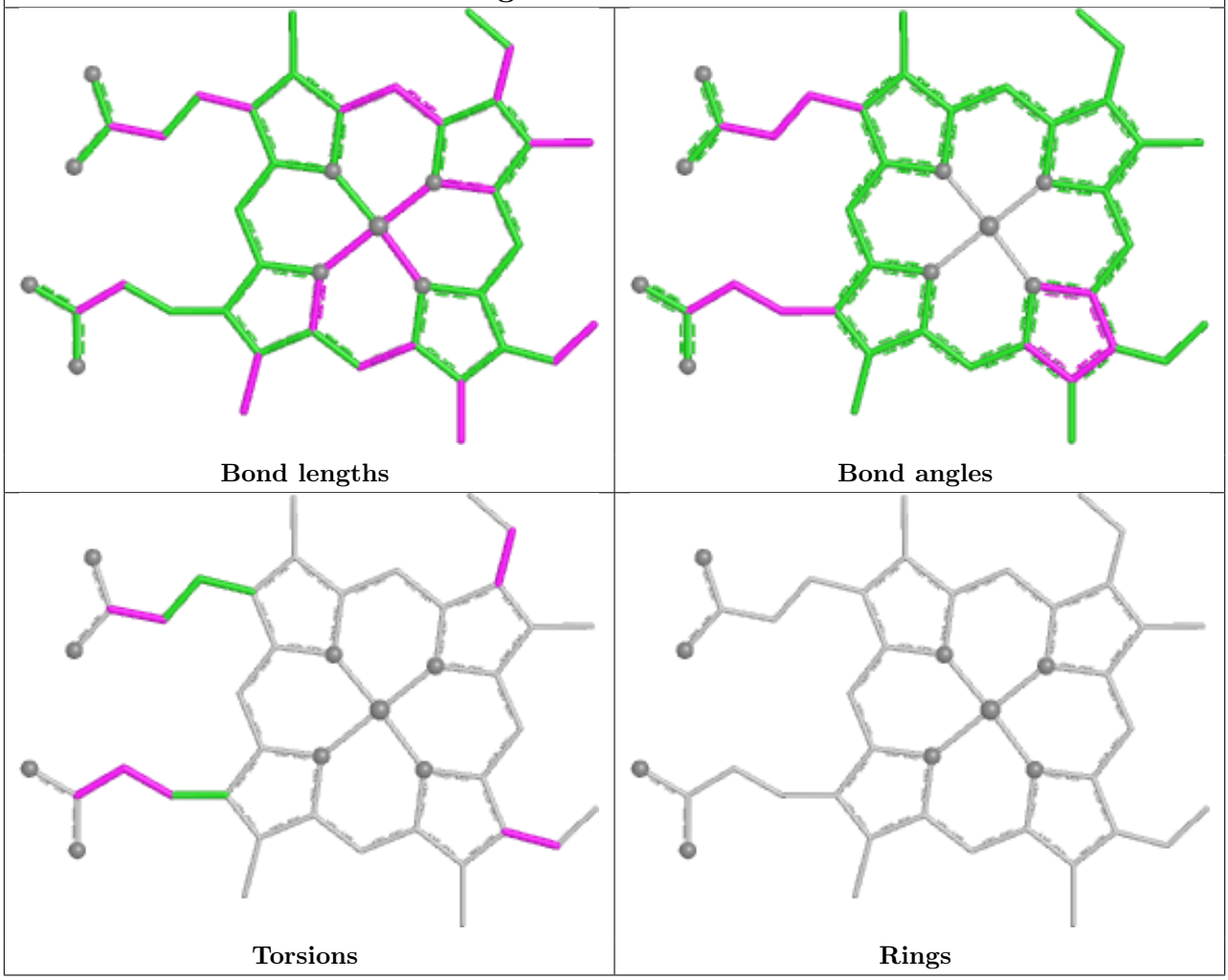


Torsions



Rings

Ligand HEM B 404



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	373/406 (91%)	-0.34	3 (0%)	82	71	13, 41, 81, 100	0
1	B	374/406 (92%)	-0.27	4 (1%)	78	65	16, 42, 85, 100	0
All	All	747/812 (91%)	-0.31	7 (0%)	81	68	13, 42, 82, 100	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	403	GLY	3.0
1	B	381	GLY	2.8
1	B	246	GLY	2.3
1	A	57	GLU	2.1
1	A	380	GLY	2.1
1	B	402	GLU	2.1
1	B	403	GLY	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

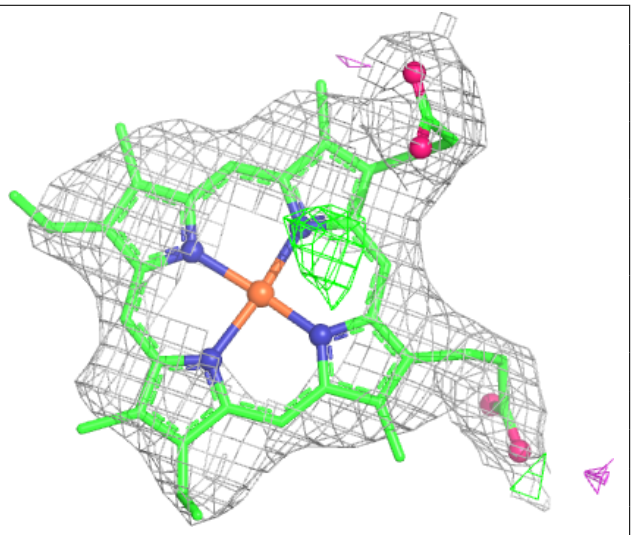
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

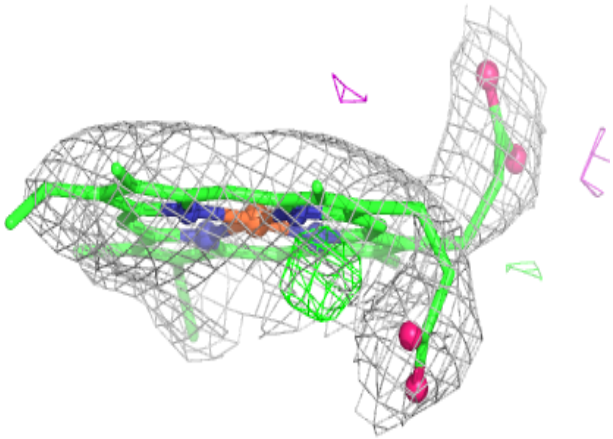
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NHE	A	407	13/13	0.67	0.23	82,95,100,100	0
4	NHE	A	406	13/13	0.83	0.17	64,74,94,95	0
4	NHE	B	1406	13/13	0.84	0.18	51,79,100,100	0
4	NHE	B	1407	13/13	0.85	0.21	70,94,100,100	0
2	CYN	A	405	2/2	0.94	0.13	31,31,31,37	0
2	CYN	B	1405	2/2	0.97	0.09	31,31,31,38	0
3	HEM	A	404	43/43	0.98	0.08	15,27,39,54	0
3	HEM	B	404	43/43	0.98	0.08	17,27,41,51	0

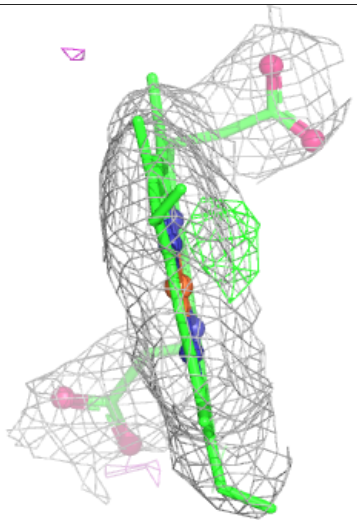
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around HEM A 404:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

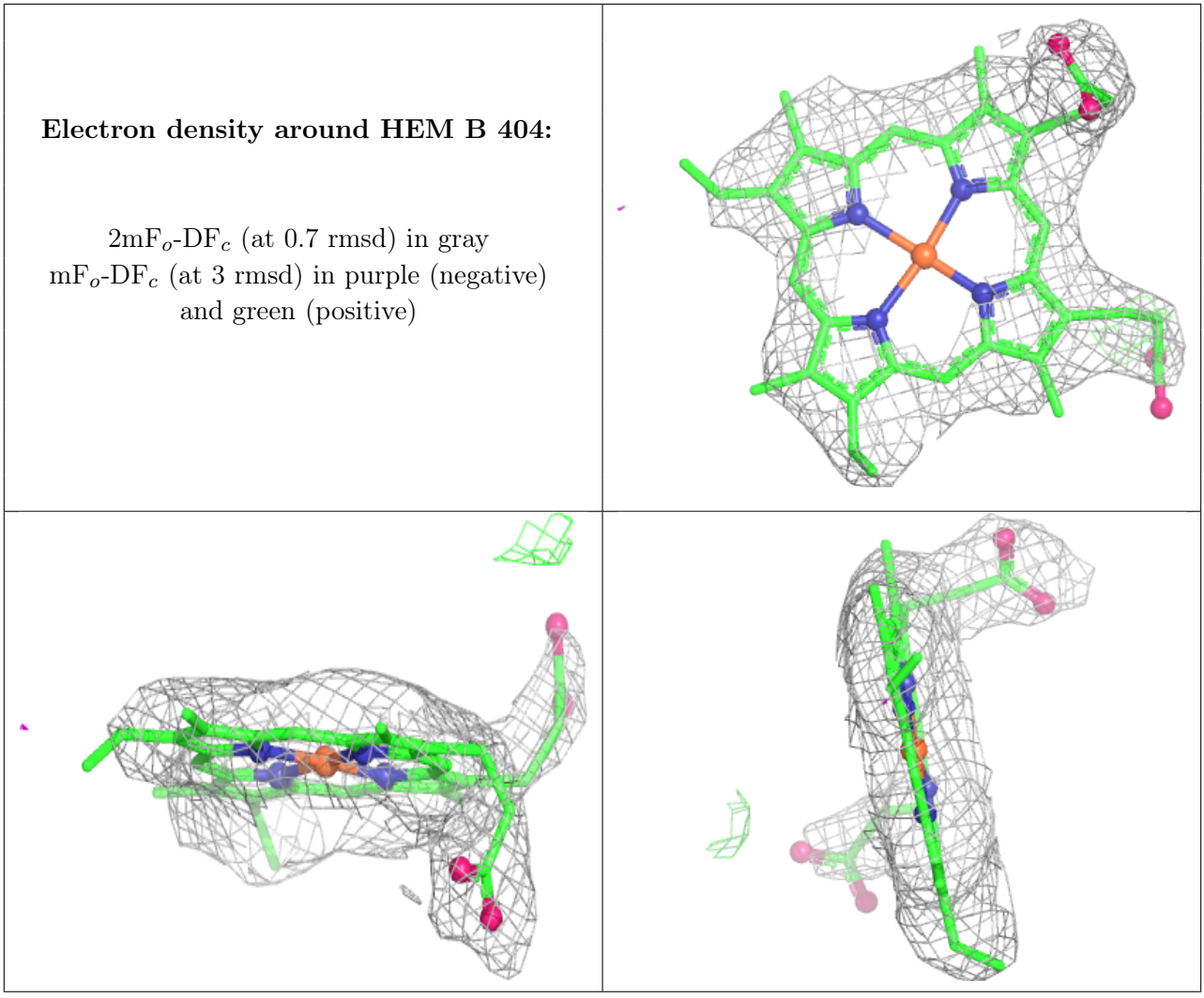






Electron density around HEM B 404:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.